

# Variation in displacement energies due to isospin nonconserving forces

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For mirror nuclei with masses  $A = 42 - 95$ , the effects of isospin nonconserving nuclear forces are studied with nuclear shell model using the Coulomb displacement energy and triplet displacement energy as probes. It is shown that the characteristic behavior of the displacement energies can be well reproduced if the isovector and isotensor nuclear interactions with  $J = 0$  and  $T = 1$  are introduced into the  $f_{7/2}$  shell. These forces, with their strengths being found consistent with the nucleon-nucleon scattering data, tend to modify nuclear binding energies near the  $N = Z$  line. At present, no evidence is found that these forces are needed for the upper  $fp$ -shell. Theoretical one- and two-proton separation energies are predicted accordingly, and locations of the proton drip-line are thereby suggested.

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Isospin is a fundamental concept in particle and nuclear physics [1]. Isospin-symmetry breaking occurs in particle physics because of the  $u$ - $d$  quark mass difference and the electromagnetic effects in quarks [2]. In nuclear physics, nucleon-nucleon scattering data suggest that the neutron-neutron ( $nn$ ) interaction is  $\sim 1\%$  more attractive than the proton-proton ( $pp$ ) interaction and the proton-neutron ( $pn$ ) interaction is  $\sim 2.5\%$  stronger than the average of the  $nn$  and  $pp$  interactions [3–5]. In nuclei, the Coulomb interaction between protons also breaks both charge symmetry and charge independence. The Coulomb displacement energy (CDE), i.e. the binding-energy difference between mirror nuclei, is a well-known signature of charge-symmetry breaking due to the Coulomb interaction [6]. However, it was realized [7] that even if the pairing, exchange, and electromagnetic spin-orbit terms are considered, the Coulomb force alone cannot account for the experimental CDE (known as the Nolen-Schiffer anomaly). There have been many attempts to resolve this discrepancy [8]. Shell-model calculations suggested that the isospin non-conserving (INC) nuclear interactions are important for understanding the anomaly [9]. In addition, one could also study the triplet displacement energy (TDE) [10], which is regarded as a measure of breaking in charge independence [6].

The study of proton-rich nuclei is one of the frontiers in low-energy nuclear physics. Proton-rich nuclei with masses  $A \sim 60 - 70$  are of particular interest. In this mass region, there are at least three so-called waiting-points along the suggested path of rapid proton capture process (the  $rp$ -process) [11]:  $^{64}\text{Ge}$ ,  $^{68}\text{Se}$ , and  $^{72}\text{Kr}$ , having equal numbers of neutrons and protons ( $N = Z$ ). Precise masses in the vicinity of the waiting-point nuclei [12–17] are required to locate the  $rp$ -process path and to understand astronomical observations on the abundance of chemical elements. The concept of CDE is thought to be a reliable method for predictions of unknown masses (or nuclear binding energies) on the proton-rich side of the  $N = Z$  line [18, 19]. In addition,  $N \sim Z$  nuclei with  $A \sim 80$  are known [20] to undergo dramatic changes in shape

[21, 22] with addition or removal of just one or two nucleons [23], which would strongly influence the determination of the end point of the  $rp$ -process [24], i.e. the heaviest element that the  $rp$ -process nucleosynthesis may create.

The CDE for mirror nuclei is defined as

$$\text{CDE}(A, T) = BE(T, T_{z<}) - BE(T, T_{z>}), \quad (1)$$

where  $T_z = (N - Z)/2$  is the  $z$  component of the total isospin  $T$ , and  $BE(T, T_{z<})$  and  $BE(T, T_{z>})$  are (negative) binding energies in an isospin multiplet having the largest proton number ( $Z_{>}$ ) and the smallest one ( $Z_{<}$ ), respectively. For  $T = 1/2$ , the experimental CDE's [15, 25] are shown in Fig. 1(a) and compared with the Coulomb energy prediction [6]. A monotonous increasing trend in CDE with increasing mass number is described for the entire region from  $A = 5$  to 71. However, an overall overestimate by the calculation is seen in Fig. 1(a). These deviations from data can be qualitatively understood by the exchange effects due to the Pauli Principle, which keeps the protons apart, thus weakening the Coulomb repulsion [6, 7]. A close examination on the curve indicates a zigzag behavior in these CDE's. To see the zigzag pattern more clearly, we introduce a quantity measuring the differences in CDE between nuclei  $A$  and  $A + 2$ ,

$$\Delta\text{CDE}(A, T) = \text{CDE}(A + 2, T) - \text{CDE}(A, T). \quad (2)$$

In Fig. 1(b), one clearly sees an odd-even staggering pattern. The Coulomb energy prediction gives only the average with a smooth curve. A notable exception in the pattern is seen for the  $f_{7/2}$ -shell nuclei with masses  $A = 42 - 52$ , where the staggering seems to be washed out considerably.

The TDE with  $T = 1$  is defined with binding energies of triplet nuclei as

$$\text{TDE}(A, T) = BE(T, T_{z<}) + BE(T, T_{z>}) - 2BE(T, T_z = 0). \quad (3)$$

In Fig. 1(c), the known experimental TDE's [25] are shown for different masses. Except for those around  $A = 6$  and at

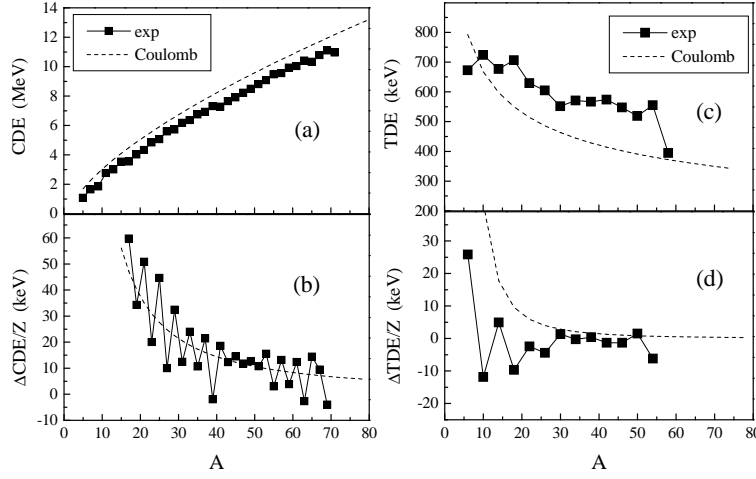


FIG. 1: Experimental Coulomb displacement energy and triplet displacement energy. (a) CDE, (b) differences in CDE between  $A$  and  $A + 2$  nuclei (shown as  $\Delta\text{CDE}/Z$ ), (c) TDE, and (d) differences in TDE between  $A$  and  $A + 4$  nuclei (shown as  $\Delta\text{TDE}/Z$ ). Experimental data are taken from Ref. [15, 25]. Theoretical curves from the Coulomb prediction [6] are shown for comparison.

$A = 58$ , the Coulomb energy prediction disagrees strongly with data, particularly for those  $f_{7/2}$ -shell nuclei where much enhanced TDE's are observed experimentally. We may further introduce a quantity measuring the differences in TDE,

$$\Delta\text{TDE}(A, T) = \text{TDE}(A + 4, T) - \text{TDE}(A, T). \quad (4)$$

In Fig. 1(d), it is seen that staggering occurs only for light nuclei, but fades away for heavier ones. For nuclei starting from  $A = 30$ , the experimental  $\Delta\text{TDE}$ 's show a smooth behavior, with only  $A = 54$  as an exception.

Questions arise as to why in the mass region of  $A = 42 - 54$  the staggering magnitude in  $\Delta\text{CDE}$  is greatly reduced, why the overall TDE is significantly larger than the Coulomb prediction for this mass region, and why the  $\Delta\text{TDE}$  at  $A = 54$  (and TDE at  $A = 58$ ) suddenly deviates from the smooth trend. To find an answer, we perform state-of-the-art shell-model calculations with inclusion of the INC interaction  $H_{\text{INC}}$  in addition to the original isoscalar Hamiltonian  $H_0$ . For  $H_0$ , we adopt two modern interactions: GXPF1A [26] with the full  $fp$  shell and JUN45 [27] with the  $pf_{5/2}g_{9/2}$  model space. The total Hamiltonian then reads

$$H = H_0 + H_{\text{INC}}, \quad (5)$$

where  $H_{\text{INC}}$  takes the form of a spherical tensor of rank two

$$H_{\text{INC}} = H'_{sp} + V_C + \sum_{k=1}^2 V_{\text{INC}}^{(k)}, \quad (6)$$

with  $V_C$  in Eq. (6) being the Coulomb interaction and  $H'_{sp}$  the single-particle Hamiltonian that includes the Coulomb single-particle energy for protons and the single-particle energy shifts  $\epsilon_{ls}$  due to the electromagnetic spin-orbit interaction for both protons and neutrons with the parameters taken from Ref. [28]. The Coulomb single-particle energies for protons are taken as (all in MeV)  $\epsilon(0f_{7/2}) = 7.4$ ,  $\epsilon(1p_{3/2}) = 7.2$ ,

$\epsilon(0f_{5/2}) = 7.1$ , and  $\epsilon(1p_{1/2}) = 7.3$  for the  $fp$  model space, and  $\epsilon(1p_{3/2}) = 9.4$ ,  $\epsilon(1f_{5/2}) = 9.1$ ,  $\epsilon(1p_{1/2}) = 10.0$ , and  $\epsilon(0g_{9/2}) = 9.7$  for the  $pf_{5/2}g_{9/2}$  model space. The electromagnetic spin-orbit term has been shown to play an important role for understanding the anomalies in the Coulomb energy difference in  $^{67}\text{As}/^{67}\text{Se}$  [29] and  $^{70}\text{Br}/^{70}\text{Se}$  [30]. The  $\epsilon_{ll}$  term [31] does not appear explicitly because this term shifts only the proton single-particle energies and are effectively included in the Coulomb single-particle energies listed above.  $V_{\text{INC}}^{(k)}$  in (6) is the INC interaction, with  $k = 1$  and  $k = 2$  for the isovector and isotensor component, respectively. The two-body matrix elements with  $T = 1$  are related to those in the proton-neutron formalism [6, 18] through

$$V_{\text{INC}}^{(1)} = V_{pp} - V_{nn}, \quad V_{\text{INC}}^{(2)} = V_{pp} + V_{nn} - 2V_{pn}, \quad (7)$$

where  $V_{pp}$ ,  $V_{nn}$ , and  $V_{pn}$  are, respectively, the  $pp$ ,  $nn$ , and  $pn$  matrix elements of  $T = 1$ .

Calculations are performed for odd-mass nuclei with isospin  $T = 1/2, 3/2$ , and  $5/2$  and for even-mass nuclei with  $T = 1, 2$ , and  $3$ , in both the  $fp$  and  $pf_{5/2}g_{9/2}$  model spaces. Because of large dimensions involved in the calculation, it is necessary to restrict the number of nucleons to be excited from the lower to the upper orbits. We have carefully checked the results between calculations with and without restrictions and found that they differ by only a few keV.

In the GXPF1A calculation within the full  $fp$  shell, the INC interaction for the  $f_{7/2}$  shell has terms (see Eq. (7))  $V_{pp} = \beta_{pp}V_{pp}^{J=0}$ ,  $V_{nn} = \beta_{nn}V_{nn}^{J=0}$ , and  $V_{pn} = \beta_{pn}V_{pn}^{J=0}$ , where  $V_{pp}^{J=0}$ ,  $V_{nn}^{J=0}$ , and  $V_{pn}^{J=0}$  are, respectively, the  $pp$ ,  $nn$ , and  $pn$  pairing interactions for the matrix elements having a unit value. The parameters  $\beta_{pp} = -22.5$ ,  $\beta_{nn} = 77.5$ , and  $\beta_{pn} = -55.0$  (all in keV) are chosen so as to reproduce the experimental CDE and TDE data. Fig. 2(a) shows that the calculated CDE with and without the INC interaction can describe the experimen-

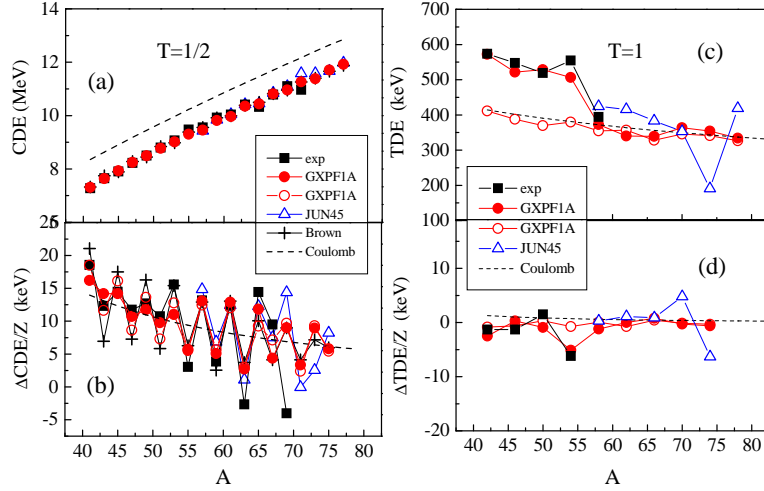


FIG. 2: (Color online) Calculations with GXPFI1A and JUN45 interactions are compared with experimental data [15, 25] for (a) CDE, (b)  $\Delta\text{CDE}(A, T)/Z$ , (c) TDE, and (d)  $\Delta\text{TDE}(A, T)/Z$ . Solid (open) symbols indicate results with (without) the INC nuclear interactions in the  $f_{7/2}$  shell. For comparison, results from Brown *et al.* [19] and from the Coulomb prediction [6] are also shown.

tal data reasonably well. However, we find that only with the isovector and isoscalar interactions can the calculation correctly reproduce the observed reduction in staggering magnitude of  $\Delta\text{CDE}/Z$  for the mass region  $A = 45 - 51$ , as shown in Fig. 2(b), and the large experimental TDE shown in Fig. 2(c). Without the INC nuclear interaction, the calculated staggering magnitudes for  $\Delta\text{CDE}/Z$  are clearly larger than the data and the TDE values are close to the Coulomb prediction, but smaller by about 150 keV than the experiment. In the JUN45 calculation, the INC interaction is not included.

The underlying physics is that inclusion of the isovector force in the  $f_{7/2}$  shell modifies interactions between the nucleons. Namely,  $pp$  ( $nn$ ) now becomes more attractive (less attractive), which results in an increase (decrease) of the proton (neutron) pairing gap. To see its influence on  $\Delta\text{CDE}$  directly, we rewrite Eq. (2) as

$$\Delta\text{CDE}(A, T) = 2(-1)^{Z_{>}} [\Delta_{\pi}(Z_{>}, Z_{>}) - \Delta_{\nu}(Z_{>}, Z_{>})], \quad (8)$$

in which  $\Delta_{\nu}(Z_{>}, Z_{>})$  and  $\Delta_{\pi}(Z_{>}, Z_{>})$  are the three-point odd-even mass differences for neutrons and protons, respectively, which are regarded as measures of the neutron- and proton-pairing gap [32]. The occurrence of the odd-even staggering can then be explained by the differences between proton- and neutron-pairing gaps, with the factor  $(-1)^{Z_{>}}$  originating from number parity. Without the isovector force in the  $f_{7/2}$  shell, calculations give an overly strong staggering for  $A = 43 - 51$  (see Fig. 2(b)). Now with inclusion of the isovector force, an increasing difference between  $\Delta_{\pi}$  and  $\Delta_{\nu}$  is obtained. With  $Z_{>} = \text{odd (even)}$ , the factor  $(-1)^{Z_{>}}$  in Eq. (8) is negative (positive) for  $A = 41, 45, \dots$  ( $A = 43, 47, \dots$ ). As compared to the results without the isovector force, this obviously leads to a decrease in  $\Delta\text{CDE}$  for the sequence with odd  $Z_{>}$  and an increase for even  $Z_{>}$ , thus reproducing the observed reduction of staggering magnitudes shown in Fig. 2(b). On the other

hand, since inclusion of the isoscalar force makes  $pn$  more attractive than the average of  $pp$  and  $nn$ , the last term in Eq. (3) becomes smaller, thus increasing the TDE for  $A = 42 - 54$ , as shown in Fig. 2(c). We note that the calculations do not support the apparent change in the staggering phase at  $A = 69$  in the experimental  $\Delta\text{CDE}$ . This may suggest [33] that the mass of  $^{69}\text{Br}$  [16] was measured for an isomer, not for the ground state. From the present calculations, we find that  $nn$  is  $\sim 0.8\%$  more attractive than  $pp$ , and  $pn$  is  $\sim 2.5\%$  stronger than the average of  $nn$  and  $pp$ . These ratios are in accord with those estimated from the nucleon-nucleon scattering data [4].

For the heavier mass region with  $A = 55 - 67$ , the calculated CDE differences are also in a good agreement with the observed large staggering (see Fig. 2(b)). The sudden drop in TDE at  $A = 58$  (Fig. 2(c)) and the corresponding drop in  $\Delta\text{TDE}$  at  $A = 54$  (Fig. 2(d)) are correctly reproduced. For nuclei below  $A = 54$ , since nucleons occupy mainly the  $f_{7/2}$  shell, the added INC interaction shows a significant effect, which correctly describes the observed large TDE, as discussed above. For the triplet nuclei with  $A = 58$ , however, two nucleons occupy the  $p_{3/2}$  orbit and do not feel an INC interaction, and therefore, the TDE decreases drastically. Thus, in our calculation the observed sudden drop in TDE at  $A = 58$  may suggest that the INC nuclear interaction is less important for the normal-parity  $p_{3/2}$  and  $f_{5/2}$  orbits. Differences between the GXPFI1A and JUN45 calculations are found above  $A = 69$  in Fig. 2, which are attributed to the contribution from the  $g_{9/2}$  orbit.

On the basis of the successful CDE calculation as presented in Fig. 2, now we try to map the proton drip-line by evaluating one- and two-proton separation energies. According to Eq. (1), we use the shell-model CDE and the observed binding energy  $BE(T, T_{z_{>}})$  for the nucleus from the neutron-rich side to predict the binding energy  $BE(T, T_{z_{<}})$  for the proton-rich ana-

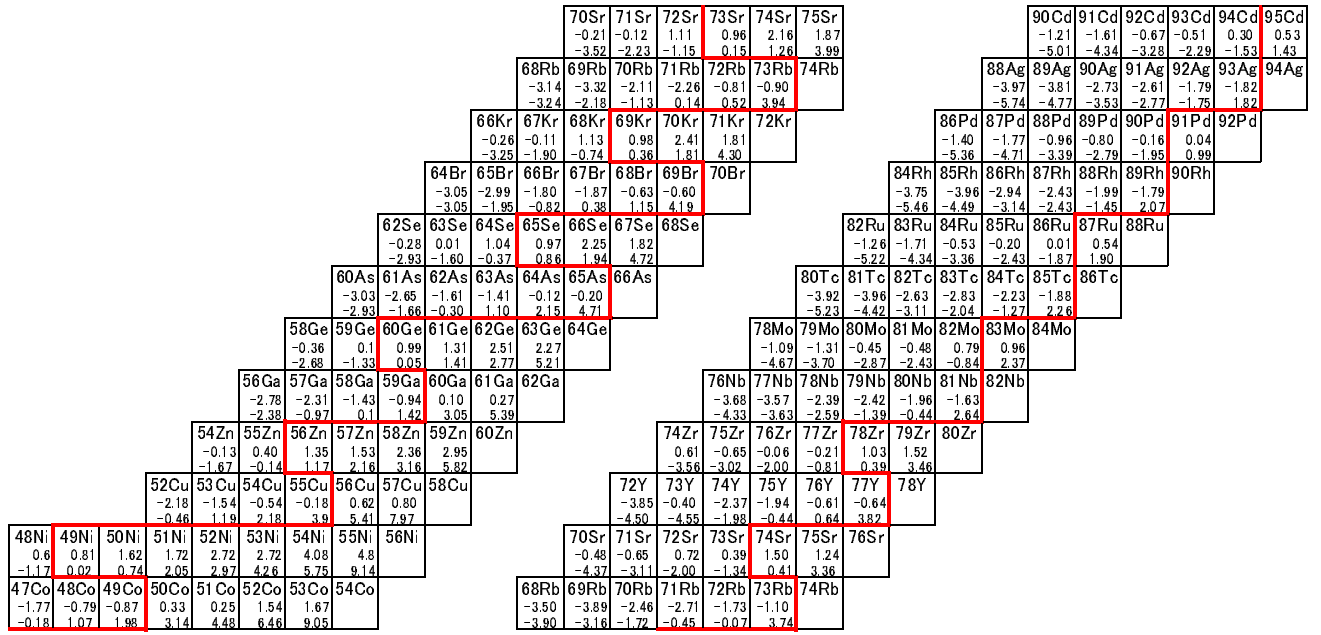


FIG. 3: (Color online) Calculated one- and two-proton separation energies for odd-mass nuclei with isospin  $T = 1/2, 3/2, 5/2$  and for even-mass nuclei with  $T = 1, 2, 3$  using the GXPF1A (left) and the JUN45 (right) interaction. In each box, the first number denotes one-proton separation energy and the second denotes two-proton separation energy. Thick (red) lines indicate the proton drip-line.

logue nucleus. For binding energies above  $A = 82$  where no data are available, we simply adopt the Audi-Wapstra extrapolation from AME'03 [25]. The agreement between the calculated and experimental binding energies is very good within an rms deviation of about 100 keV. Figure 3 shows the calculated one- and two-proton separation energies denoted in each box by the first and second numbers, respectively. The thick (and red) lines represent the proton drip-line beyond which the one-proton and/or two-proton separation energies become negative. The INC term for the  $f_{7/2}$  shell is included in the calculation with the GXPF1A interaction. The existing data for  $^{60}\text{Ga}$  [12],  $^{64,65}\text{As}$  [15, 17], and  $^{69}\text{Br}$  [13, 16] indicate that these nuclei are unbound. The experimental separation energies of  $^{63}\text{Ge}$ ,  $^{67}\text{Se}$ , and  $^{71}\text{Kr}$  [15] suggest that they are bound. In the graph on the right, the experiments indicate that  $^{77}\text{Y}$  and  $^{82}\text{Mo}$  are bound while no evidence was found for  $^{81}\text{Nb}$  and  $^{85}\text{Tc}$ . As one can see, most of our results are consistent with the current experimental information. Figure 3 also suggests several candidates for proton emitters.

In summary, we have investigated effects of the isospin nonconserving forces that cause characteristic shell changes near the  $N = Z$  line. Large-scale shell-model calculations were performed by employing two modern effective interactions (GXPF1A and JUN45) for the corresponding mass regions with inclusion of the Coulomb plus INC nuclear interactions. We concluded that the INC forces are important for the  $f_{7/2}$ -shell nuclei, but not for the upper  $fp$ -shell. This conclusion is consistent with those found in our previous papers [29, 30]. No conclusion about the INC forces can currently be drawn for heavier nuclei with  $A = 70 - 95$ . Consequently,

we calculated one- and two-proton separation energies to map the proton drip-line. Our calculation provides many new predictions for the  $fpg$  shell region up to  $A = 95$ , which may be relevant to the discussion of the  $rp$ -process of nucleosynthesis [24]. The results shown in the present Letter should be tested by future experiments on proton-rich nuclei of the heavy mass region.

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